class06_HW

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Q6. How would you generalize the original code above to work with any set of input protein structures?

Write your own function starting from the code above that analyzes protein drug interactions by reading in any protein PDB data and outputs a plot for the specified protein.

Create a new RMarkdown document with your function code AND example output. We also suggest you include narrative text that address the rubric items below. Generate a PDF report and submit this PDF to our GradeScope site

Here is the starting code:

```
# Can you improve this analysis code?
library(bio3d)
s1 <- read.pdb("4AKE")  # kinase with drug
```

```
  Note: Accessing on-line PDB file
```

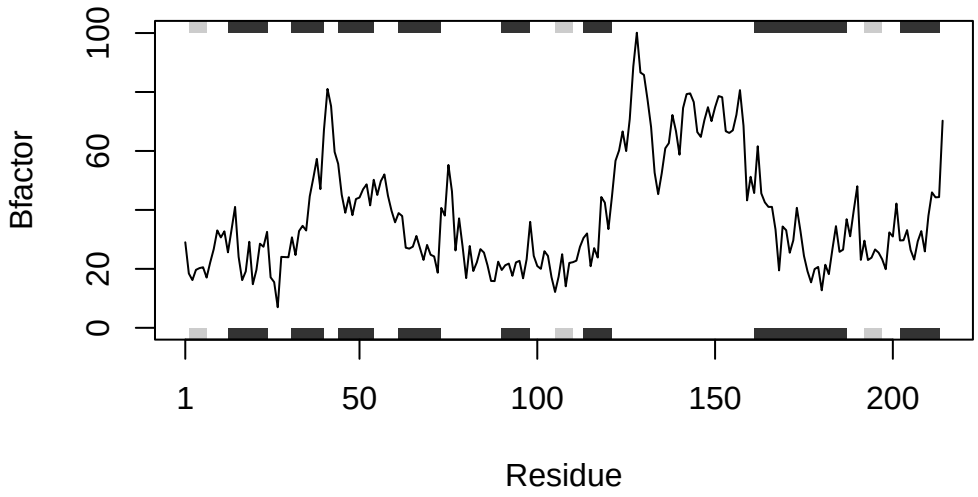
```
s2 <- read.pdb("1AKE")  # kinase no drug
```

```
  Note: Accessing on-line PDB file
   PDB has ALT records, taking A only, rm.alt=TRUE
```

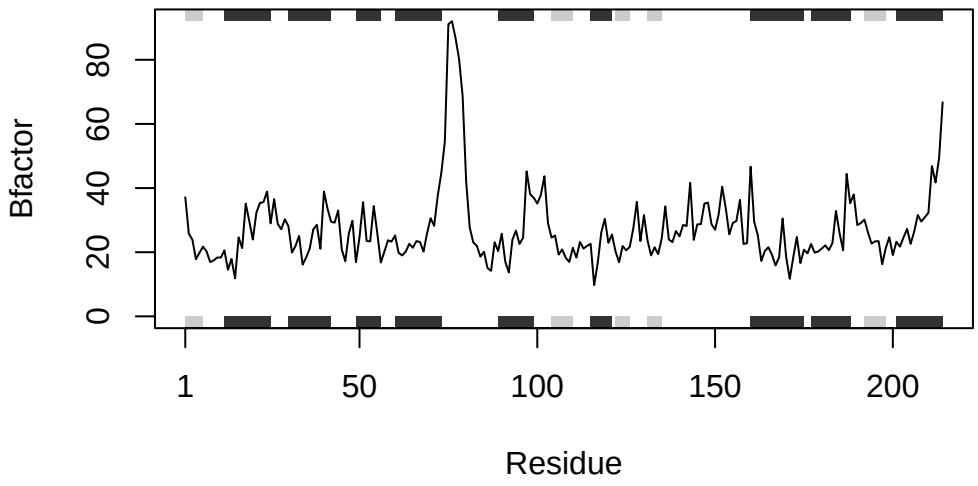
```
s3 <- read.pdb("1E4Y")  # kinase with drug
```

```
  Note: Accessing on-line PDB file
```

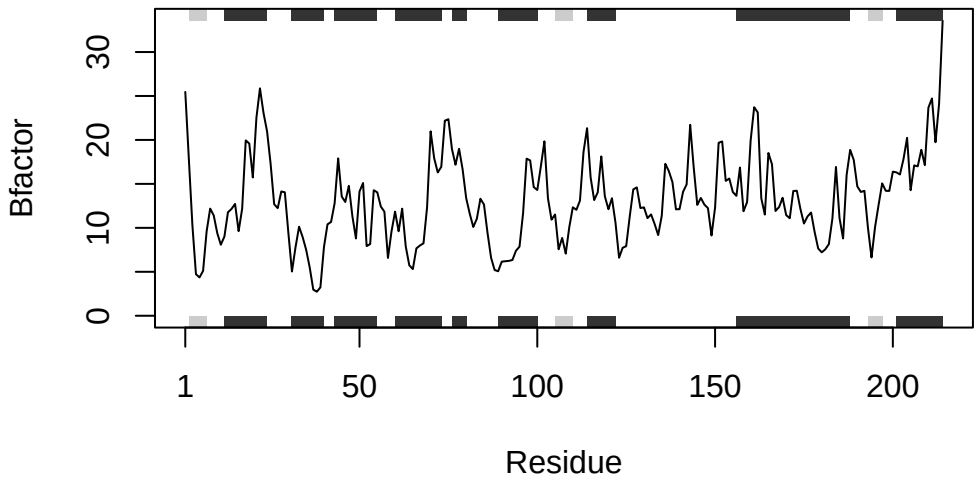
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
s3.chainA <- trim.pdb(s3, chain="A", elety="CA")
s1.b <- s1.chainA$atom$b
s2.b <- s2.chainA$atom$b
s3.b <- s3.chainA$atom$b
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```




```
plotb3(s2.b, sse=s2.chainA, typ="l", ylab="Bfactor")
```




```
plotb3(s3.b, sse=s3.chainA, typ="l", ylab="Bfactor")
```



Re-writing the code to make it a function that can work with any set of input protein structures:

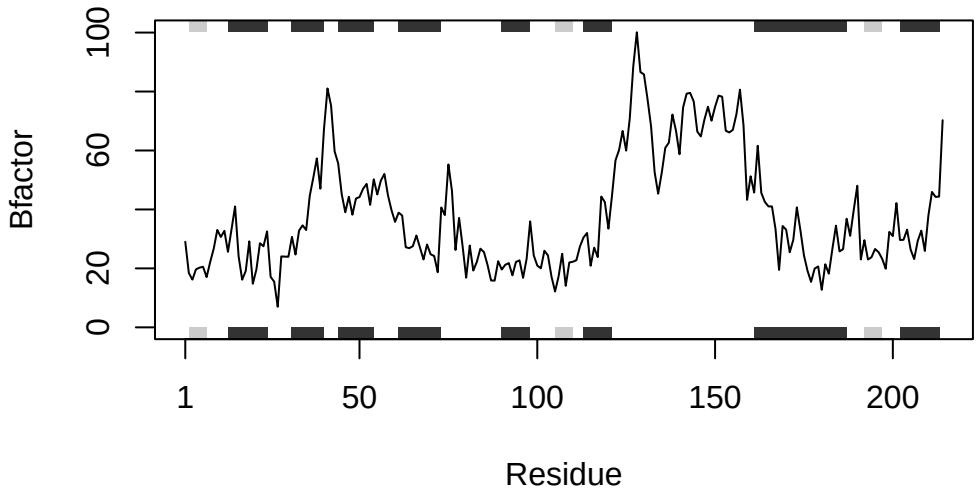
```r
#plot_bfactor is a function that plots the b factor for a given protein structure,
#which can give insights on the relative flexability/rigidity of the protein

#plot_bfactor takes in a pdb code for a protein as well as an optional chain
#parameter that is default set to chain A, but can be changed if the user
#specifies.
plot_bfactor <- function(pdb_code, prot_chain = "A") {

  #the structure of the protein is read in a as a pdb file using the input pdb
  #code
  structure <- read.pdb(pdb_code)

  #the alpha carbons of the desired protein chain within the protein structure
  #are selected. if the user specified the protein chain then it would be used
  #here, or else chain A is used as default
  structure.chain <-  trim.pdb(structure, chain=prot_chain, elety="CA")

  #the b factor values for the atoms selected in the previous step are selected
  #here
  structure.bfactor <- structure.chain$atom$b

  #a scatter plot of the b factor value for each atom in the protein structure
  #is created. this is the output of the function
  plotb3(structure.bfactor, sse=structure.chain, typ="l", ylab="Bfactor")
}
```

Calling the function plot_bfactor to test it:

```r
s1 = "4AKE"
plot_bfactor(s1)
```

```
  Note: Accessing on-line PDB file
```

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
C:\Users\iruud\AppData\Local\Temp\RtmpQDs5Ch/4AKE.pdb exists. Skipping download
```

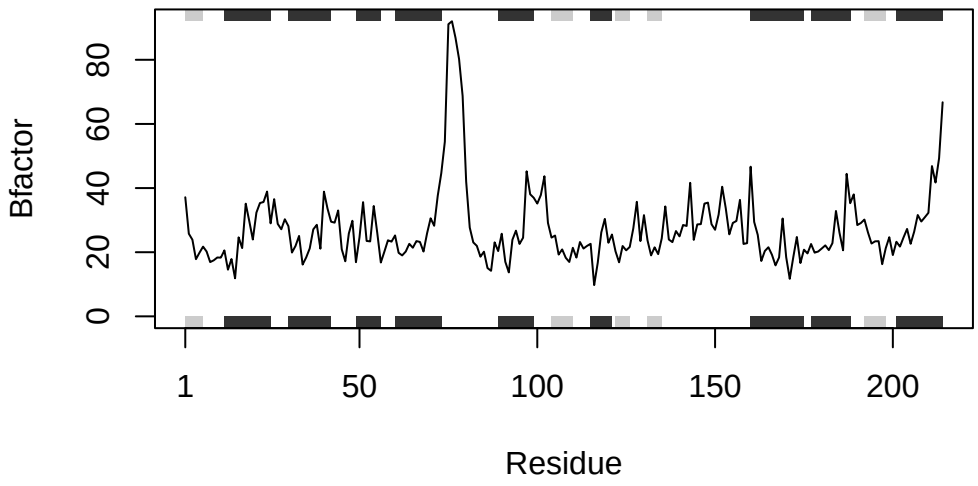



```
s2 = "1AKE"
plot_bfactor(s2)
```

```
  Note: Accessing on-line PDB file
```

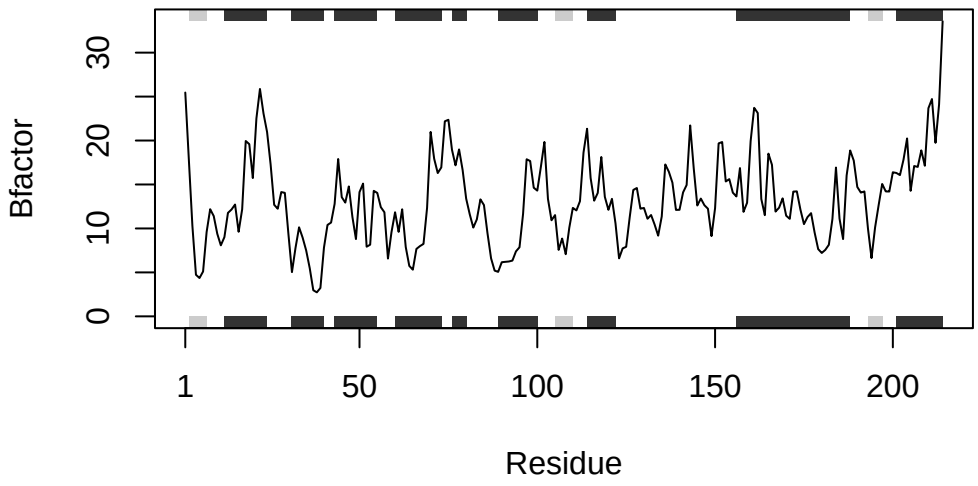
```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
C:\Users\iruud\AppData\Local\Temp\RtmpQDs5Ch/1AKE.pdb exists. Skipping download
```

```
   PDB has ALT records, taking A only, rm.alt=TRUE
```




```
s3 = "1E4Y"
plot_bfactor(s3)
```

```
  Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
C:\Users\iruud\AppData\Local\Temp\RtmpQDs5Ch/1E4Y.pdb exists. Skipping download
```

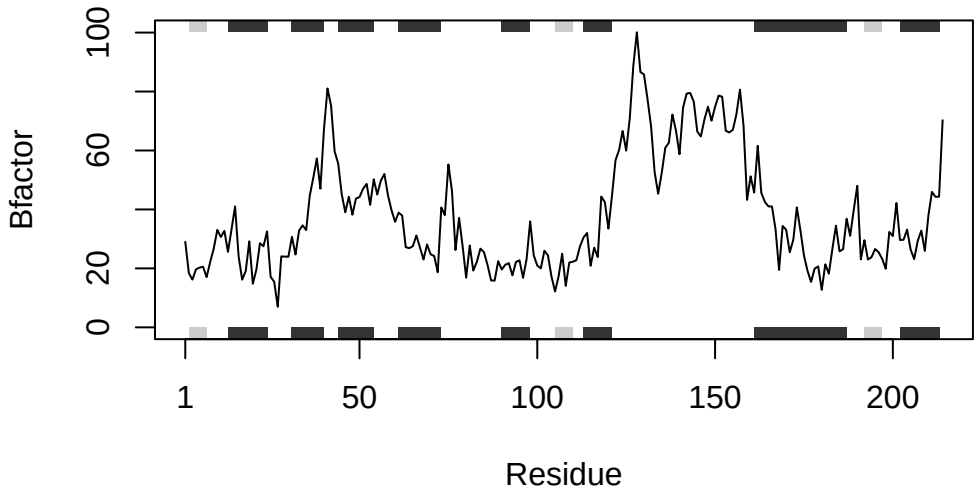


Applying function to a list of structures:

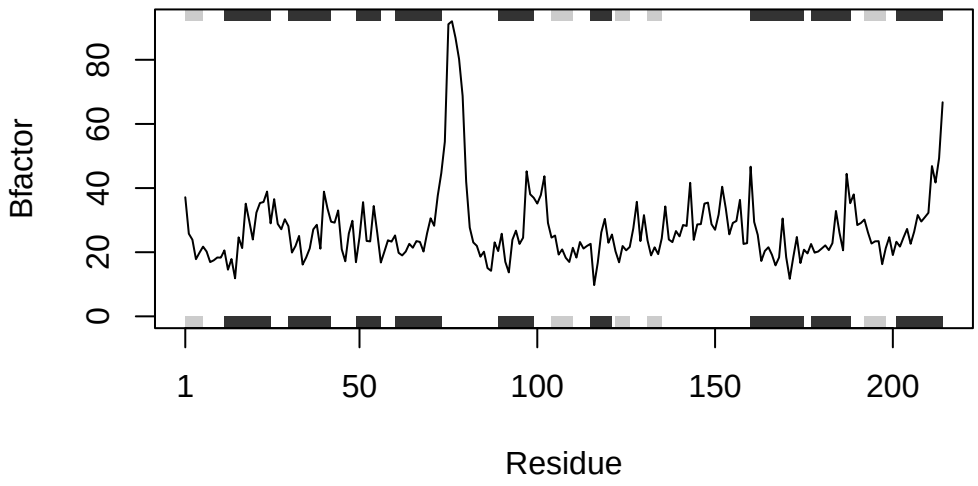
```
s1 = "4AKE"
s2 = "1AKE"
s3 = "1E4Y"
structures <- c(s1,s2,s3)
sapply(structures, plot_bfactor)
```

```
  Note: Accessing on-line PDB file
```

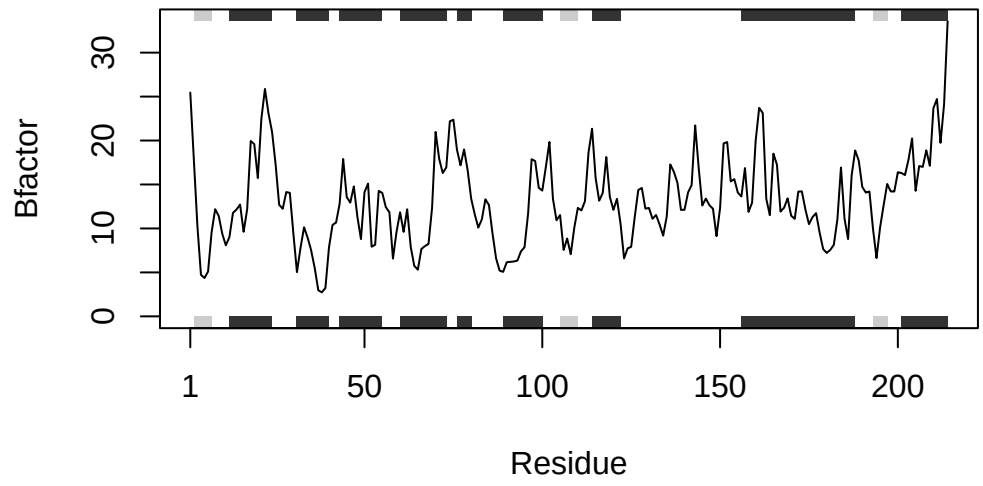
```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
C:\Users\iruud\AppData\Local\Temp\RtmpQDs5Ch/4AKE.pdb exists. Skipping download
```




```
  Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
C:\Users\iruud\AppData\Local\Temp\RtmpQDs5Ch/1AKE.pdb exists. Skipping download

   PDB has ALT records, taking A only, rm.alt=TRUE
```




```
  Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
C:\Users\iruud\AppData\Local\Temp\RtmpQDs5Ch/1E4Y.pdb exists. Skipping download
```




```
$`4AKE`
NULL

$`1AKE`
NULL

$`1E4Y`
NULL
```